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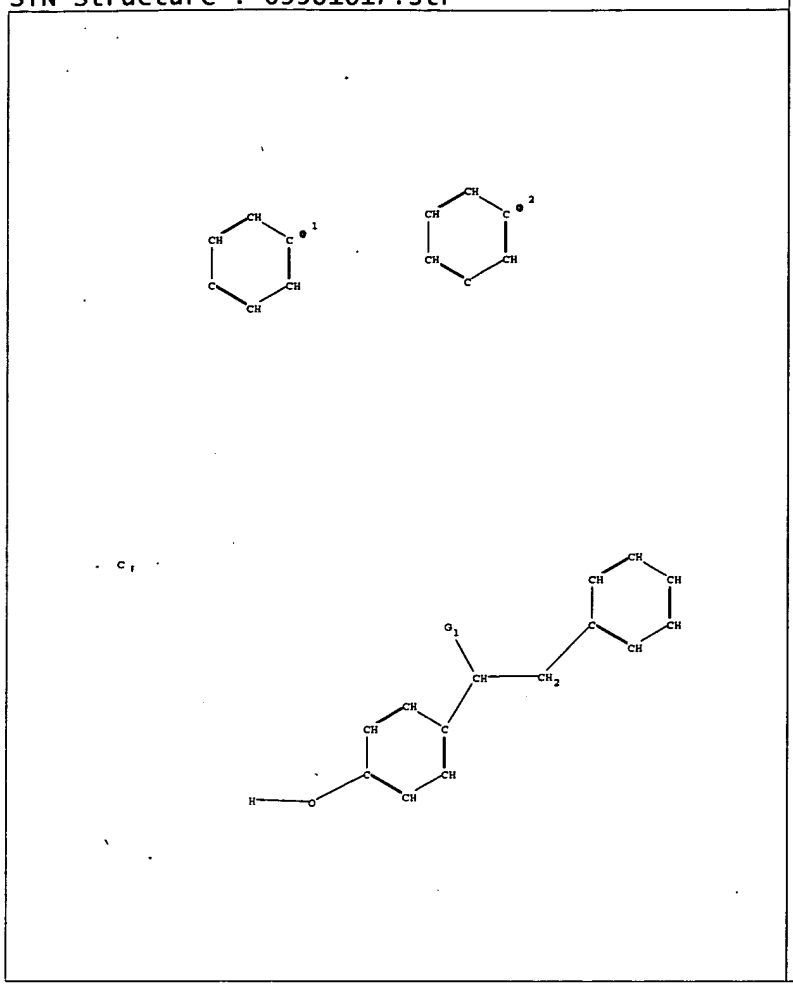

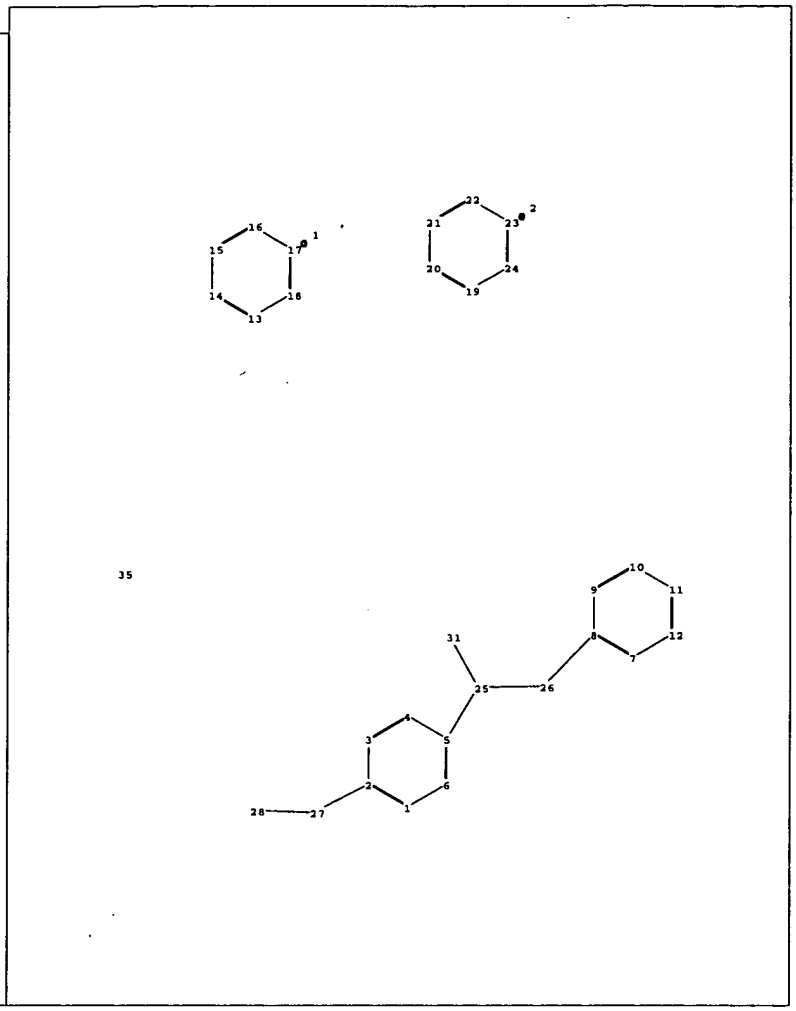

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ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
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ring bonds :
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15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
2-27 25-31
exact bonds :
5-25 8-26 25-26 27-28
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
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G1:[*1],[*2]

Hydrogen count :
14:>=0 19:>=0
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     FILE 'REGISTRY' ENTERED AT 11:52:24 ON 30 SEP 2002
L1                SCREEN 1006
L2                STRUCTURE UPLOADED
L3                QUE L2 AND L1
L4              0 S L3 SSS SAM
L5              8 S L3 SSS FULL

     FILE 'CAPLUS' ENTERED AT 11:53:01 ON 30 SEP 2002
L6             10 S L5
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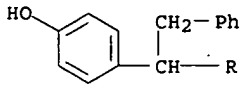
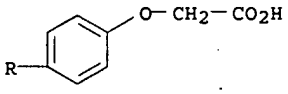
L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:863500 CAPLUS
DOCUMENT NUMBER: 136:5799
TITLE: Preparation of triarylethanes as estrogen mimetics lacking reproductive tract effects
INVENTOR(S): Ruenitz, Peter C.
PATENT ASSIGNEE(S): The Univeristy of Georgia Research Foundation, Inc., USA
SOURCE: U.S., 19 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6323190	B1	20011127	US 1999-363911	19990728
US 2002045664	A1	20020418	US 2001-981617	20011015

PRIORITY APPLN. INFO.: US 1998-94944P P 19980731
US 1999-363911 XX 19990728
OTHER SOURCE(S): MARPAT 136:5799
AB A method for treating symptoms, diseases and conditions in extra-reproductive tract tissues that are responsive to treatment with estrogen, using triarylethanes I [R1 = O(CH2)mR3, (CH2)nR3; R3 = anionic substituent; m = 1 to 4; n = 0 to 4; R2 = H, OH], is reported. E.g., a multistep synthesis of 4-[1-(p-hydroxyphenyl)-2-phenylethyl]phenoxyacetic acid was prepd. from PhCH2OC6H4CHO-4 and 4-BrC6H4OH.
IT **185223-83-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of triarylethanes as estrogen mimetics lacking reproductive tract effects)
RN 185223-83-0 CAPLUS
CN Acetic acid, [4-[1-(4-hydroxyphenyl)-2-phenylethyl]phenoxy]- (9CI) (CA INDEX NAME)





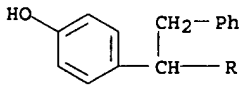
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

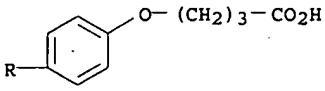
L6 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:426033 CAPLUS
DOCUMENT NUMBER: 135:282668
TITLE: Identification of new triarylethylene oxyalkanoic acid analogues as bone selective estrogen mimetics
AUTHOR(S): Rubin, V. N.; Ruenitz, P. C.; Boudinot, F. D.; Boyd, J. L.
CORPORATE SOURCE: College of Pharmacy, University of Georgia, Athens, GA, 30602-2352, USA
SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(6), 1579-1587
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Previously, the estrogen receptor (ER) ligand 4-[1-(p-hydroxyphenyl)-2-phenylethyl]phenoxyacetic acid (I) was found to have differential bone

loss suppressive effects in the ovariectomized (OVX) rat approaching those of selective ER modulators (SERMs) such as tamoxifen. In an effort to improve efficacy, analogs of this compd. were prepd. which incorporated features designed to reduce polarity/ionizability. Thus, the acetic acid side chain of I was replaced by n-butanoic acid and 1H-tetrazol-4-ylmethyl moieties. Also, the phenolic hydroxyl of I was replaced. We also developed new methods for the synthesis of triarylethylene variants. In the OVX rat, 4-{[1-(p-hydroxyphenyl)-2-phenyl-1-butenyl]phenoxy}-n-butanoic acid and its des-hydroxy counterpart were as effective as 17.beta.-estradiol in suppressing serum markers of bone resorption/turnover, namely osteocalcin and deoxypyridinoline, but had only 30% of the uterotrophic efficacy of 17.beta.-estradiol. This study has thus identified two triarylethylene oxybutyric acids that have differential bone/uterus effects like those of known SERMs. These oxybutyric acids have been found to have an activity profile similar to established selective estrogen receptor modulators (SERMs) with significant bone protecting effects and minimal uterotrophic activity.

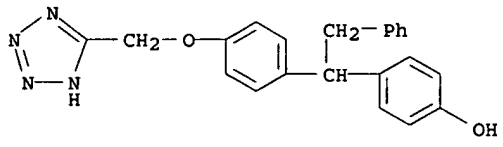
IT **364635-57-4P 364635-59-6P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(triarylethylene oxyalkanoic acid analogs as bone selective estrogen mimetics)

RN 364635-57-4 CAPLUS
CN Butanoic acid, 4-[4-[1-(4-hydroxyphenyl)-2-phenylethyl]phenoxy]- (9CI) (CA INDEX NAME)



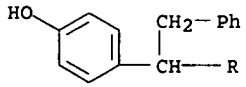


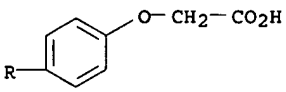
RN 364635-59-6 CAPLUS
CN Phenol, 4-[2-phenyl-1-[4-(1H-tetrazol-5-ylmethoxy)phenyl]ethyl]- (9CI) (CA INDEX NAME)



IT **185223-83-0**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(triarylethylene oxyalkanoic acid analogs as bone selective estrogen mimetics)

RN 185223-83-0 CAPLUS
CN Acetic acid, [4-[1-(4-hydroxyphenyl)-2-phenylethyl]phenoxy]- (9CI) (CA INDEX NAME)





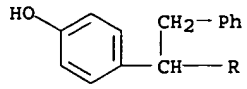
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

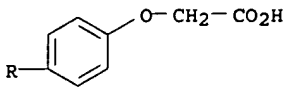
L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:5748 CAPLUS
DOCUMENT NUMBER: 130:232431
TITLE: Specific bone-protective effects of metabolites/derivatives of tamoxifen and clomiphene in ovariectomized rats
AUTHOR(S): Ruenitz, P. C.; Shen, Y.; Li, M.; Liang, H.; Whitehead, R. D., Jr.; Pun, S.; Wronski, T. J.
CORPORATE SOURCE: College of Pharmacy, University of Georgia, Athens, GA, 30602, USA
SOURCE: Bone (New York) (1998), 23(6), 537-542
CODEN: BONEDL; ISSN: 8756-3282
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In the ovariectomized (ovx) rat, the nonsteroidal antiestrogens, clomiphene (CLO) and tamoxifen (TAM), at dose levels that prevent development of osteopenia to a degree approaching that of 17.beta.-estradiol are, in contrast to 17.beta.-estradiol, only weakly uterotrophic. Metabolites of CLO and TAM might contribute differentially to these effects. Thus, we have evaluated bone protective and uterine effects in ovx rats of two such metabolites: 4-hydroxy CLO, produced by p-hydroxylation of CLO; and 4HTA, produced from TAM by stepwise replacement of its dimethylaminoethyl side chain with an acetic acid moiety, accompanied by p-hydroxylation. Also reported are effects of D4HTA, the dihydrodesethyl deriv. of 4HTA previously characterized as a full estrogen mimetic in vitro. Administration of 4-hydroxy CLO (2.5 mg/kg s.c.) 5 days/wk for 5 wk to 3-mo old ovx rats resulted in complete prevention of bone loss and suppression of bone turnover to levels comparable to those of intact controls and to those of ovx animals similarly receiving 17.beta.-estradiol (10 .mu.g/kg). However, uterine wt. in animals receiving 4-hydroxy CLO was 64% less than that in 17.beta.-estradiol-treated animals. Although 4HTA (3.7 mg/kg s.c.) had a modest uterotrophic effect, it did not prevent bone loss assocd. with ovariectomy. In contrast, D4HTA (3.6 mg/kg s.c.) partially reduced bone turnover indicators and cancellous bone loss in a manner similar in many ways to that obsd. in TAM-treated ovx animals, but it had no uterotrophic effect. These results suggest that, although 4HTA does not contribute to the bone-protective effect of TAM, 4-hydroxy CLO might augment that of CLO.

IT **185223-83-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tamoxifen and clomiphene metabolites/derivs. specific bone-protective effects in ovariectomy)

RN 185223-83-0 CAPLUS
CN Acetic acid, [4-[1-(4-hydroxyphenyl)-2-phenylethyl]phenoxy]- (9CI) (CA INDEX NAME)



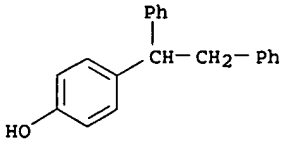


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:253139 CAPLUS
DOCUMENT NUMBER: 128:229915
TITLE: Radical Chemistry under Diffusional Constraints: Impact of Spacer Molecules on the Thermolysis of Surface-Immobilized Bibenzyl
AUTHOR(S): Buchanan, A. C. III; Britt, Phillip F.; Thomas, Kimberly B.
CORPORATE SOURCE: Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831-6197, USA
SOURCE: Energy & Fuels (1998), 12(3), 649-659
CODEN: ENFUEM; ISSN: 0887-0624
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Silica nanoparticle surfaces have been chem. modified to contain a mol. probe, 1,2-diphenylethane (bibenzyl), as well as a second spacer mol. of variable structure. Thermolysis kinetics and products at 400 .degree.C have been detd. for bibenzyl, and the impact of diffusional constraints and spacer mol. structure on the multipathway radical chem. has been analyzed relative to fluid phases. Unimol. homolysis rate consts., k = (7-9) .times. 10-6 s-1, are found to be independent of spacer mol. structure (naphthalene, diphenylmethane, tetralin) and similar to values measured in fluid phases, indicating the lack of a cage effect on the silica surface. However, the total rate of bibenzyl thermolysis and the resulting product selectivities are profoundly affected by both surface immobilization and the structure of the spacer mol. Naphthalene spacers behave as "mol. walls" serving as phys. barriers to bimol. hydrogen transfer steps on the surface and augmenting the effects of diffusional constraints. In contrast, diphenylmethane spacers are found to serve as hydrogen transfer, radical relay catalysts that translocate radical sites across the surface and diminish the impact of diffusional constraints. Tetralin spacers undergo significant reaction with free-radical intermediates, selectively producing the isomeric methylindan via a chain pathway that is promoted by the restrictions on diffusion.

IT **205396-63-0D**, silica immobilized
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); FORM (Formation, nonpreparative); PROC (Process)
(radical chem. under diffusional constraints the impact of spacer mols. on thermolysis of surface-immobilized bibenzyl)
RN 205396-63-0 CAPLUS
CN Phenol, 4-(1,2-diphenylethyl)- (9CI) (CA INDEX NAME)



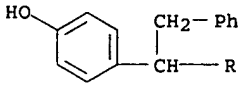
L6 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:67392 CAPLUS
DOCUMENT NUMBER: 128:201102
TITLE: Estrogenic tamoxifen derivatives: categorization of

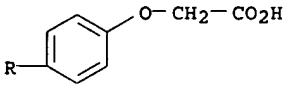
intrinsic estrogenicity in MCF-7 cells
AUTHOR(S): Ruenitz, Peter C.; Moore, Susan A.; Kraft, Kelly S.; Bourne, Caryl S.
CORPORATE SOURCE: College of Pharmacy, University of Georgia, Athens, GA, 30602-2352, USA
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1997), 63(4-6), 203-209
CODEN: JSBBEZ; ISSN: 0960-0760
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Triarylethylenes bearing acetic acid side chains, exemplified by 4-[1-(p-hydroxyphenyl)-2-phenyl-1-butenyl]phenoxyacetic acid (4HTA), a deriv. of tamoxifen (TAM), are of current interest as estrogen mimics lacking reproductive tract effects. Affinities for estrogen receptors (ER) and effects on cell growth kinetics of a diverse series of such compds. were compared with 4HTA, TAM, and with std. estrogens 17.beta.-estradiol (E2) and chlorotrianisene (CTA) in MCF-7 cells. These compds. exhibited concn. dependent cell growth stimulation comparable to that of CTA but less than that of E2. Growth stimulation of the more potent compds. was antagonized by TAM, signifying that effects were mediated via interaction with ER. At concns. of 1 .mu.M or higher, compds. with efficacies less than that of E2 were weak antagonists of estradiol-stimulated growth. Both intracellular ER affinities and growth rate stimulation potencies of the triarylethylene acetic acids and the std. ER ligands varied over a range of nearly three orders of magnitude. Anal. of growth stimulatory potency as a function of ER affinity revealed dual parallel correlations: the potency/ER affinity ratios of 4HTA and four of its analogs was about 100-fold less than those of the hydroxytriarylethane and bisphenolic analogs and the three std. ER ligands. These results suggested that ER liganded with the latter substances is more 'effective' at nuclear effector sites than is ER liganded with 4HTA and the other acidic triarylethylenes.

IT **185223-83-0**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(estrogenic tamoxifen derivs. and categorization of intrinsic estrogenicity in MCF-7 cells)

RN 185223-83-0 CAPLUS
CN Acetic acid, [4-[1-(4-hydroxyphenyl)-2-phenylethyl]phenoxy]- (9CI) (CA INDEX NAME)





L6 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:286454 CAPLUS
DOCUMENT NUMBER: 126:268327
TITLE: UV-shielding colorants coated with polyarylates for cosmetics
INVENTOR(S): Tanaka, Takumi
PATENT ASSIGNEE(S): Daito Kasei Kogyo Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 09052819	A2	19970225	JP 1995-203671	19950809

AB Title colorants are coated with polyarylates I (R1, R2 = alkyl, ally, aryl; n .gtoreq. 5). Sericite was dispersed in a CH2Cl2 soln. contg. polyarylate [from 2,2-bis(4-hydroxyphenyl)propane, terephthalic acid, and isophthalic acid], mixed with MeOH, filtered, dried, and pulverized to prep. a colorant powder showing good transparency and UV absorbability.

IT **188796-13-6**
RL: BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(UV-shielding colorants coated with polyarylates for cosmetics)

RN 188796-13-6 CAPLUS

CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid and 4,4'-(2-phenylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

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CRN 4052-96-4
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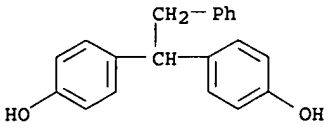
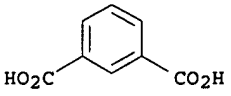


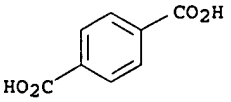
CM 2

CRN 121-91-5
CMF C8 H6 O4



CM 3

CRN 100-21-0
CMF C8 H6 O4



L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:286453 CAPLUS
DOCUMENT NUMBER: 126:268326
TITLE: UV-shielding cosmetics containing polyarylates
INVENTOR(S): Tanaka, Takumi
PATENT ASSIGNEE(S): Daito Kasei Kogyo Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09052818	A2	19970225	JP 1995-203670	19950809

AB Title cosmetics, which show transparency and good UV absorbability, contain polyarylates I (R1, R2 = alkyl, allyl, aryl; n .gtoreq. 5) or colorants coated with I. Talc, TiO2, sericite, mica, and iron oxides were dispersed in a CH2Cl2 soln. of polyarylate [prepd. from 2,2-bis(4-hydroxyphenyl)propane, terephthalic acid, and isophthalic acid] to prep. polyarylate-coated colorants. A pressed powder foundation was formulated from the talc 54.0, the TiO2 5.0, the sericite 27.9, the mica 5.0, the red iron oxide 0.5, the yellow iron oxide 1.0, the black iron oxide 0.1, lanolin 1.0, liq. paraffin 3.5, iso-Pr myristate 2.0 wt. parts, antioxidant, and antiseptic to 100 parts.

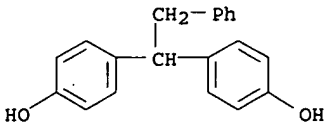
IT **188796-13-6**
RL: BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(UV-shielding cosmetics contg. polyarylates)

RN 188796-13-6 CAPLUS

CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid and 4,4'-(2-phenylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

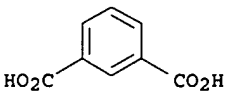
CM 1

CRN 4052-96-4
CMF C20 H18 O2



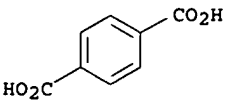
CM 2

CRN 121-91-5
CMF C8 H6 O4



CM 3

CRN 100-21-0
CMF C8 H6 O4



L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:758884 CAPLUS
DOCUMENT NUMBER: 126:24858
TITLE: Photoresist with photoactive compound mixture
INVENTOR(S): Zampini, Anthony; Trefonas, Peter, III; Turci, Pamela; Meister, Catherine C.; Vizvary, Gerald C.
PATENT ASSIGNEE(S): Shipley Company, L.L.C., USA
SOURCE: Eur. Pat. Appl., 31 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 737895	A1	19961016	EP 1996-103151	19960301
EP 737895	B1	19990908		
R: DE, FR, GB, IT				
JP 08286370	A2	19961101	JP 1996-87843	19960410
US 5723254	A	19980303	US 1996-706096	19960904

PRIORITY APPLN. INFO.: US 1995-419099 19950410

AB The invention relates to a pos.-acting photoresist compn. contg. a mixt. of photoactive compds. One component of the mixt. is the esterification product of an o-quinonediazidesulfonyl compd. with a phenolic resin. Another component of the mixt. is the esterification product of an o-quinonediazidesulfonyl compd. with a low-mol.-wt. phenol having from one to three aryl groups and from one to three hydroxyl groups. A third component which may be present in the formulation is the esterification product of an o-quinonediazidesulfonyl compd. with a relative high-mol.-wt., polyhydric, polynuclear phenol.

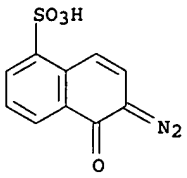
IT **184489-94-9**
RL: TEM (Technical or engineered material use); USES (Uses)
(pos. photoresists contg. phenolic resin quinonediazidosulfonates and)

RN 184489-94-9 CAPLUS

CN 1-Naphthalenesulfonic acid, 6-diazo-5,6-dihydro-5-oxo-, ester with 4,4'-(2-phenylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

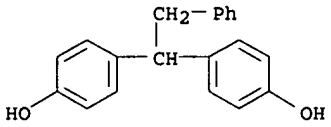
CM 1

CRN 20546-03-6
CMF C10 H6 N2 O4 S



CM 2

CRN 4052-96-4
CMF C20 H18 O2



L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2002 ACS

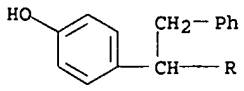
ACCESSION NUMBER:	1996:656497 CAPLUS
DOCUMENT NUMBER:	126:69720
TITLE:	Estrogenic Triarylethylene Acetic Acids: Effect of Structural Variation on Estrogen Receptor Affinity and Estrogenic Potency and Efficacy in MCF-7 Cells
AUTHOR(S):	Ruenitz, Peter C.; Bourne, Caryl S.; Sullivan, Kelly J.; Moore, Susan A.
CORPORATE SOURCE:	College of Pharmacy, University of Georgia, Athens, GA, 30602-2352, USA
SOURCE:	Journal of Medicinal Chemistry (1996), 39(24), 4853-4859 CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER:	American Chemical Society
DOCUMENT TYPE:	Journal
LANGUAGE:	English

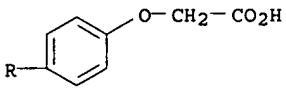
AB Triarylethylenecarboxylic acids exemplified by (E,Z)-2-{4-[1-(p-hydroxyphenyl)-2-phenyl]-1-butenyl}phenoxyacetic acid (I) are a new class of estrogen receptor (ER) ligands capable of tissue selective estrogen agonist and antagonist effects. We report the syntheses of I and of analogs incorporating structural features known or anticipated to facilitate ER affinity in triarylethylenes. These studies revealed that the p-hydroxyphenyl moiety, ethylenic bond, and ether oxygen of I were all crit. for high estrogen receptor ER affinity. Although a 1,1-bisphenolic analog bearing the p-(oxyacetic acid) moiety on its 2-Ph ring, 12, had low ER affinity, it exhibited estrogenic potency approaching that of I in MCF-7 cells. Unlike I which was a partial agonist with weak antagonist potency, II was a full agonist. A similar profile of potency/efficacy in MCF-7 cells was seen in 9, an ethylenic bond satd. analog of I. Growth-promoting effects of I and II were fully antagonized by the antiestrogen tamoxifen, suggesting that such effects were mediated solely via ER. Thus, our studies in MCF-7 cells have confirmed the estrogenicity of I and have enabled identification of two analogs with favorable estrogenic potency and full estrogen efficacy. On this basis, these three (triarylethylene)acetic acids have been selected for more intensive animal studies of their extrareproductive tract estrogenic effects. drug resistance.

IT **185223-83-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and structure activity relations of triarylethylenecarboxylic acids for estrogen receptor affinity and estrogenic potency and efficacy in MCF-7 cells)

RN 185223-83-0 CAPLUS

CN Acetic acid, [4-[1-(4-hydroxyphenyl)-2-phenylethyl]phenoxy]- (9CI) (CA INDEX NAME)





L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:103083 CAPLUS

DOCUMENT NUMBER: 118:103083

TITLE: Effect of articulated side groups on the main-chain flexibility of polycarbonates

AUTHOR(S): Sundararajan, P. R.

CORPORATE SOURCE: Xerox Res. Cent. Canada, Mississauga, ON, L5K 2L1, Can.

SOURCE: Macromolecules (1993), 26(2), 344-8
CODEN: MAMOBX; ISSN: 0024-9297

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Conformational energies are calcd. for a series of polycarbonates with articulated side groups attached to the central C.alpha. atom. In all the cases considered, the placement of a CH2 spacer for the articulated side chain increases the main-chain rigidity as compared to that of bisphenol A polycarbonate although the energies of the segment at the min. are lowered. The min. also become localized, thus impeding the synchronous rotation of the phenyls within a low energy barrier. A new steric factor based on the conformational partition function is used for comparing the chain flexibilities. The cases of the articulated side chains deviate from the correlation between the conformational entropy and glass temp. which applies for the homologous series of polycarbonates with nonarticulated side groups.

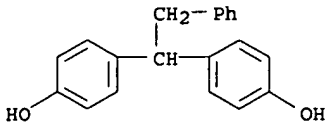
IT **146066-21-9**
RL: PRP (Properties)
(flexibility of main chain of, effect of side group on)

RN 146066-21-9 CAPLUS

CN Carbonic acid, polymer with 4,4'-(2-phenylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

CRN 4052-96-4
CMF C20 H18 O2



CM 2

CRN 463-79-6
CMF C H2 O3